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* * * * * Welcome to STN International * * * * *

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NEWS 1          Web Page for STN Seminar Schedule - N. America
NEWS 2 DEC 01    ChemPort single article sales feature unavailable
NEWS 3 JAN 06    The retention policy for unread STNmail messages
                  will change in 2009 for STN-Columbus and STN-Tokyo
NEWS 4 JAN 07    WPIDS, WPINDEX, and WPIX enhanced Japanese Patent
                  Classification Data
NEWS 5 FEB 02    Simultaneous left and right truncation (SLART) added
                  for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS 6 FEB 02    GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS 7 FEB 06    Patent sequence location (PSL) data added to USGENE
NEWS 8 FEB 10    COMPENDEX reloaded and enhanced
NEWS 9 FEB 11    WTEXTILES reloaded and enhanced
NEWS 10 FEB 19   New patent-examiner citations in 300,000 CA/CAPLUS
                  patent records provide insights into related prior
                  art
NEWS 11 FEB 19   Increase the precision of your patent queries -- use
                  terms from the IPC Thesaurus, Version 2009.01
NEWS 12 FEB 23   Several formats for image display and print options
                  discontinued in USPATFULL and USPAT2
NEWS 13 FEB 23   MEDLINE now offers more precise author group fields
                  and 2009 MeSH terms
NEWS 14 FEB 23   TOXCENTER updates mirror those of MEDLINE - more
                  precise author group fields and 2009 MeSH terms
NEWS 15 FEB 23   Three million new patent records blast AEROSPACE into
                  STN patent clusters
NEWS 16 FEB 25   USGENE enhanced with patent family and legal status
                  display data from INPADOCDB
NEWS 17 MAR 06   INPADOCDB and INPAFAMDB enhanced with new display
                  formats
NEWS 18 MAR 11   EPFULL backfile enhanced with additional full-text
                  applications and grants
NEWS 19 MAR 11   ESBIOBASE reloaded and enhanced
NEWS 20 MAR 20   CAS databases on STN enhanced with new super role
                  for nanomaterial substances
NEWS 21 MAR 23   CA/CAPLUS enhanced with more than 250,000 patent
                  equivalents from China
NEWS 22 MAR 30   IMSPATENTS reloaded and enhanced
NEWS 23 APR 03   CAS coverage of exemplified prophetic substances
                  enhanced
NEWS 24 APR 07   STN is raising the limits on saved answers

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NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 16:56:55 ON 21 APR 2009

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=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.22	0.22

FILE 'REGISTRY' ENTERED AT 16:57:07 ON 21 APR 2009

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STRUCTURE FILE UPDATES: 20 APR 2009 HIGHEST RN 1137276-53-9

DICTIONARY FILE UPDATES: 20 APR 2009 HIGHEST RN 1137276-53-9

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<http://www.cas.org/support/stngen/stdoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10578826.str



chain nodes :
8 9 11 13
ring nodes :
1 2 3 4 5
chain bonds :
3-11 5-8 8-9 8-13
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 3-11 4-5 5-8 8-9 8-13
isolated ring systems :
containing 1 :

G1:S,CH

G2:C,N

G3:Ph,Cy,Hy

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 8:CLASS 9:CLASS 11:CLASS 13:CLASS

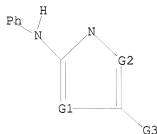
10578826

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 S,CH

G2 C,N

G3 Ph,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 16:57:24 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 26838 TO ITERATE

7.5% PROCESSED 2000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 526956 TO 546564

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 16:57:31 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 540616 TO ITERATE

100.0% PROCESSED 540616 ITERATIONS

16 ANSWERS

SEARCH TIME: 00.00.08

L3 16 SEA SSS FUL L1

=> FIL HCAPLUS

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

185.88

186.10

FILE 'HCAPLUS' ENTERED AT 16:57:46 ON 21 APR 2009

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FILE COVERS 1907 - 21 Apr 2009 VOL 150 ISS 17
FILE LAST UPDATED: 20 Apr 2009 (20090420/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 14 L3

=> s l4 and py<=2003

24035193 PY<=2003

L5 9 L4 AND PY<=2003

=> d l4 ibib abs hitstr tot

L4 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:1059573 HCAPLUS

DOCUMENT NUMBER: 147:469265

TITLE: Structure-Based Design and Synthesis of
(5-Arylamino-2H-pyrazol-3-yl)-biphenyl-2',4'-diols as
Novel and Potent Human CHK1 Inhibitors

AUTHOR(S): Teng, Min; Zhu, Jinjiang; Johnson, Michael D.; Chen,
Ping; Kornmann, Jill; Chen, Enhong; Blasina,
Alessandra; Register, James; Anderes, Kenna; Rogers,
Caroline; Deng, Yali; Ninkovic, Sacha; Grant, Stephan;
Hu, Qiyue; Lundgren, Karen; Peng, Zhengwei; Kania,
Robert S.

CORPORATE SOURCE: Department of Medicinal Chemistry, Biochemical
Pharmacology, Research Pharmacology, Crystallography
and Computational Chemistry, Pfizer Global Research
and Development, San Diego, CA, 92121-1194, USA
SOURCE: Journal of Medicinal Chemistry (2007), 50(22),
5253-5256

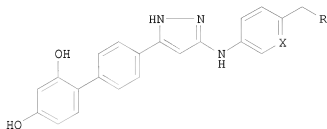
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

10578826

LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:469265
GI

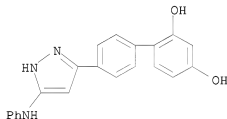


AB The cocrystal structure of a library hit was used to design a novel series of CHK1 inhibitors. The new series retained the critical hydrogen-bonding groups of the resorcinol moiety for binding but lacked the phenolic anilide moiety. The newly designed compds. I (X = CH, N; R = Me₂CHNH, Me₂N, pyrrolo, piperidino, cyclopropylamino, etc.) exhibited similar enzymic activity, while demonstrating increased cellular potency. I (X = CH, R = cyclopropylamino), showing no single agent effect, potentiated the antiproliferative effect of Gemcitabine in both prostate and breast cancer cell lines.

IT 838823-53-3P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(cocrystal structure bound to CHK1 enzyme; structure-based design and preparation of (5-arylamino-3-pyrazolyl)biphenyls as human CHK1 inhibitors)

RN 838823-53-3 HCAPLUS

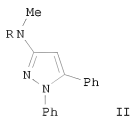
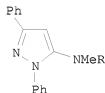
CN [1,1'-Biphenyl]-2,4-diol, 4'-[5-(phenylamino)-1H-pyrazol-3-yl]- (CA INDEX NAME)



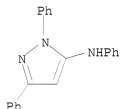
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1122125 HCAPLUS
DOCUMENT NUMBER: 144:36286
TITLE: Highly Regioselective Synthesis of 1-Aryl-3 (or 5)-alkyl/aryl-5 (or 3)-(N-cycloamino)pyrazoles
AUTHOR(S): Peruncheralathan, S.; Yadav, A. K.; Ila, H.; Junjappa, H.
CORPORATE SOURCE: Department of Chemistry, Indian Institute of

SOURCE: Technology, Kanpur, 208016, India
 Journal of Organic Chemistry (2005), 70(23), 9644-9647
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 144:36286
 GI



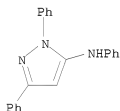
AB An efficient highly regioselective protocol for the synthesis of isomeric 1,3-diaryl (or 1-aryl-3-alkyl) and 1,5-diaryl (or 1-aryl-5-alkyl)-5 (or 3)-(N-cycloamino)pyrazoles has been reported by cyclocondensation of common α -oxoketene N,S-acetal precursors with arylhydrazines by variation of reaction conditions. E.g., reaction of $\text{PhCOCH:C(SMe)NMeCH}_2\text{C}_6\text{H}_4\text{OMe-4}$ with PhNHNH_2 in presence of NaH in DMF/ C_6H_6 gave 65% 5-aminopyrazole I ($\text{R} = \text{CH}_2\text{C}_6\text{H}_4\text{OMe-4}$). On the other hand, reaction of $\text{PhCOCH:C(SMe)NMeCH}_2\text{C}_6\text{H}_4\text{OMe-4}$ with PhNHNH_2 in presence of DABCO gave 69% 3-aminopyrazole II (same R).
 IT 94863-16-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (regioselective preparation of isomeric 1,3-diaryl (or 1-aryl-3-alkyl) and 1,5-diaryl (or 1-aryl-5-alkyl)-5 (or 3)-(N-cycloamino)pyrazoles by cyclocondensation of α -oxoketene N,S-acetal precursors with arylhydrazines)
 RN 94863-16-8 HCAPLUS
 CN 1H-Pyrazol-5-amine, N,1,3-triphenyl- (CA INDEX NAME)



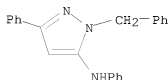
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2005:419724 HCAPLUS

DOCUMENT NUMBER: 143:115479
 TITLE: Solid-Phase Synthesis of 5-Substituted Amino Pyrazoles
 AUTHOR(S): Dodd, Dharmpal S.; Martinez, Rogelio L.; Kamau, Muthoni; Ruan, Zheming; Van Kirk, Katy; Cooper, Christopher B.; Hermsmeier, Mark A.; Traeger, Sarah C.; Poss, Michael A.
 CORPORATE SOURCE: Early Discovery Chemistry New Leads Chemistry-Applied Biotechnology and Discovery Analytical Services, Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, NJ, 08543-4000, USA
 SOURCE: Journal of Combinatorial Chemistry (2005), 7(4), 584-588
 CODEN: JCCHFF; ISSN: 1520-4766
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 143:115479
 AB An efficient method for the solid-supported synthesis of 5-N-alkylamino and 5-N-arylamino pyrazoles is described. This method is general and mild and utilizes readily accessible resin-immobilized β -ketoamides as starting materials. Resin-immobilized β -ketoamide, aryl-, or alkylhydrazine and Lawesson's reagent are suspended in a mixture of THF/Py and heated at 50-55 °C to give a resin-bound 5-aminopyrazole, that is liberated from the solid support by treatment with TFA.
 IT 94863-16-8P 857636-66-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (solid-supported synthesis of 5-N-alkylamino and 5-N-arylamino pyrazoles using resin-immobilized β -ketoamides as starting materials)
 RN 94863-16-8 HCAPLUS
 CN 1H-Pyrazol-5-amine, N,1,3-triphenyl- (CA INDEX NAME)



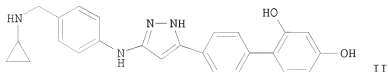
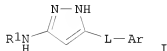
RN 857636-66-9 HCAPLUS
 CN 1H-Pyrazol-5-amine, N,3-diphenyl-1-(phenylmethyl)- (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2005:99354 HCAPLUS
 DOCUMENT NUMBER: 142:198068
 TITLE: Preparation of aminopyrazoles as CHK1 checkpoint protein kinase inhibitors.
 INVENTOR(S): Johnson, Michael David; Teng, Min; Zhu, Jinjiang
 PATENT ASSIGNEE(S): Pfizer Inc., USA
 SOURCE: PCT Int. Appl., 127 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005009435	A1	20050203	WO 2004-IB2397	20040714
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2532231	A1	20050203	CA 2004-2532231	20040714
BR 2004012820	A	20060926	BR 2004-12820	20040714
JP 2006528661	T	20061221	JP 2006-521691	20040714
US 20050043381	A1	20050224	US 2004-897849	20040722
MX 2006000933	A	20060330	MX 2006-933	20060124
PRIORITY APPLN. INFO.:			US 2003-489976P	P 20030725
			WO 2004-IB2397	W 20040714
OTHER SOURCE(S):		CASREACT 142:198068; MARPAT 142:198068		
GI				

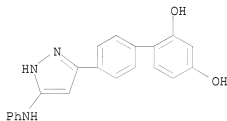


AB Title compds. [I; L = 5-6 membered (substituted) heterocyclylene; Ar = 5-6 membered (substituted) (hetero)aryl; R1 = (substituted) aryl(alkyl), heterocyclyl(alkyl), cycloalkyl(alkyl), alkenyl, alkyl; R2 = H, halo, (substituted) alkyl], were prepared Thus, title compound (II) (preparation outlined) inhibited human CHK1 with Ki <1 nM.

IT 838823-53-3P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (claimed compound; preparation of aminopyrazoles as CHK1 checkpoint protein kinase inhibitors)

RN 838823-53-3 HCAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 4'-[5-(phenylamino)-1H-pyrazol-3-yl]- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:385028 HCAPLUS

DOCUMENT NUMBER: 141:123593

TITLE: One-pot synthesis of 5-(substituted-amino)pyrazoles

AUTHOR(S): Dodd, Dharmpal S.; Martinez, Rogelio L.

CORPORATE SOURCE: Squibb Pharmaceutical Research Institute, Early Discovery Chemistry, Bristol-Myers, Princeton, NJ, 08543-4000, USA

SOURCE: Tetrahedron Letters (2004), 45(22), 4265-4267

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

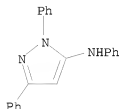
LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:123593

AB An efficient and mild one-pot synthesis of substituted 5-alkylamino and/or 5-(arylamino)pyrazoles is described. A suitably decorated β -keto amide, an aryl or alkyl hydrazine and Lawesson's reagent are suspended in THF/Py and gently heated to yield the requisite 5-aminopyrazoles. For example, the reaction of N,N-diethyl-3-oxobutanamide with (phenyl)hydrazine in the presence of Lawesson's reagent gave N,N-diethyl-3-methyl-1-phenyl-1H-pyrazol-5-amine in 95% yield. It is postulated that this method should also be easily adaptable for automated parallel synthesis.

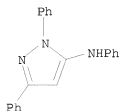
IT 94863-16-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (one-pot synthesis of pyrazolamines from β -oxo amides and hydrazines in presence of Lawesson's reagent)

RN 94863-16-8 HCAPLUS
 CN 1H-Pyrazol-5-amine, N,1,3-triphenyl- (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2002:917721 HCAPLUS
 DOCUMENT NUMBER: 138:146744
 TITLE: 1,3-Diphenyl-1H-pyrazolo[3,4-b]quinoline: A Versatile Fluorophore for the Design of Brightly Emissive Molecular Sensors
 AUTHOR(S): Rurack, Knut; Danel, Andrzej; Rotkiewicz, Krystyna; Grabka, Danuta; Spieles, Monika; Rettig, Wolfgang
 CORPORATE SOURCE: Department I.3902, Federal Institute for Materials Research and Testing (BAM), Berlin, D-12489, Germany
 SOURCE: Organic Letters (2002), 4(26), 4647-4650
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The 1,3-diphenyl-1H-pyrazolo[3,4-b]-quinoline chromophore is a versatile building block for the construction of brightly fluorescent mol. sensors. Facile synthetic procedures allow integration of the chromophore into fluorophore-spacer-receptor systems as well as fluoroionophores operating via intramol. charge transfer. Whereas the former photoinduced electron-transfer probes show strong analyte-induced fluorescence enhancement, the latter exhibit bright ratiometric dual emission. Employing prototype macrocyclic receptors, the favorable signaling features for metal ion recognition are demonstrated.
 IT 94863-16-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (1,3-di-Ph-1H-pyrazolo[3,4-b]quinoline as versatile fluorophore for design of brightly emissive mol. sensors)
 RN 94863-16-8 HCAPLUS
 CN 1H-Pyrazol-5-amine, N,1,3-triphenyl- (CA INDEX NAME)



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:545674 HCAPLUS

DOCUMENT NUMBER: 135:137516

TITLE: Synthesis of heteroarylbenzamides and analogs used for inhibiting protein kinases

INVENTOR(S): Bender, Steven Lee; Bhunalkar, Dilip; Collins, Michael Raymond; Cripps, Stephan James; Deal, Judith Gail; Nambu, Mitchell David; Palmer, Cynthia Louise; Peng, Zhengwei; Varney, Michael David; Jia, Lei

PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA

SOURCE: PCI Int. Appl., 237 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001053274	A1	20010726	WO 2001-US1723	20010119
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2394703	A1	20010726	CA 2001-2394703	20010119
US 20020103203	A1	20020801	US 2001-764306	20010119
US 6635641	B2	20031021		
EP 1252146	A1	20021030	EP 2001-906592	20010119
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001008025	A	20021105	BR 2001-8025	20010119
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MX 2002007102	A	20030128	MX 2002-7102	20020719
US 20040092747	A1	20040513	US 2003-621979	20030717
PRIORITY APPLN. INFO.:			US 2000-177059P	P 20000121
			US 2001-764306	A3 20010119
			WO 2001-US1723	W 20010119

OTHER SOURCE(S): MARPAT 135:137516

GI

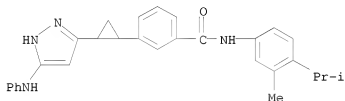
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [Z = CH, NH; Q = moiety such that ring A is (un)substituted mono- or bicyclic heteroaryl which has at least 2 carbon atoms in the heteroaryl ring system; X = CH₂, O, S, NH; Y = CH₂, O, S, provided at least one of X and Y = CH₂ or X and Y form a cyclopropyl ring; R₂-3 = H, Me, halo, CF₃, CN; R₄ = CONHR₅, NHCOR₆; where R₅ = (un)substituted aryl, heteroaryl, cycloalkyl, etc.; R₆ = (un)substituted aryl, heteroaryl, cycloalkyl, etc.] are prepared. Examples include synthetic procedures for over 150 compds., 11 biol. assays and 3 sample formulations. For instance, 3-mercaptobenzoic acid was treated with α -chloro-N-methoxy-N-methylacetamide followed by carbodiimide coupling to 2-methyl-6-aminoquinoline to give II. II was converted to a β -thiono-ketone with thioacetanilide/n-BuLi followed by treatment with hydrazine to give pyrazole III. III gave 85% inhibition of an lck protein tyrosine kinase at 5 μ M and had K_i = 2.21 nM for VEGF-R2A50. Treatment of cancer as well as other disease states associated with unwanted angiogenesis and/or cellular proliferation, such as diabetic retinopathy, neovascular glaucoma, rheumatoid arthritis, and psoriasis are claimed uses of the invention.

IT 351320-34-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (synthesis of heteroarylbenzamides used for inhibiting protein kinases)

RN 351320-34-8 HCAPLUS

CN Benzamide, N-[3-methyl-4-(1-methylethyl)phenyl]-3-[2-[5-(phenylamino)-1H-pyrazol-3-yl]cyclopropyl]- (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:673725 HCAPLUS

DOCUMENT NUMBER: 134:71524

TITLE: Microwave-assisted, facile route to 1H-pyrazolo[3,4-b]quinolines

AUTHOR(S): Danel, Andrzej; Chaczatryan, Karen; Tomasik, Piotr
 CORPORATE SOURCE: Dep. of Chem., Univ. of Agriculture, Krakow, 31 120, Pol.

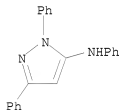
SOURCE: ARKIVOC [online computer file] (2000), 1(1), 51-57
 CODEN: AKVCFI

URL: http://www.arkat-usa.org/ARKIVOC/JOURNAL_CONTENT/manuscripts/2000/00-2107CP%20as%20published%20mainmanuscript.pdf

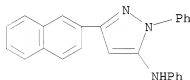
PUBLISHER: ARKAT Foundation
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:71524

AB Aromatic aldehydes have been reported to react with 5-anilinopyrazoles in the presence of ZnCl₂ to give the corresponding benzylidenopyrazoles. In this paper evidence is given that the corresponding products are, in fact, 1H-pyrazolo[3,4-b]quinolines. This observation opens a novel route to these compds. They show a blue emission in the solid state and, therefore, they are useful blue luminophores for electroluminescent devices. The synthetic procedure reported in the literature was significantly modified and improved by application of microwave heating. In our modified synthesis the reaction time was reduced from the usual 5 to 8 h to 5 to 7 min and the reaction products were formed without contamination.

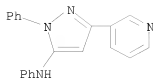
IT 94863-16-8P 314274-99-2P 314275-01-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 94863-16-8 HCAPLUS
CN 1H-Pyrazol-5-amine, N,1,3-triphenyl- (CA INDEX NAME)



RN 314274-99-2 HCAPLUS
CN 1H-Pyrazol-5-amine, 3-(2-naphthalenyl)-N,1-diphenyl- (CA INDEX NAME)



RN 314275-01-9 HCAPLUS
CN 1H-Pyrazol-5-amine, N,1-diphenyl-3-(3-pyridinyl)- (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:1287 HCAPLUS

DOCUMENT NUMBER: 124:202094

ORIGINAL REFERENCE NO.: 124:37361a,37364a

TITLE: Synthesis and biological activity of some new pyrazolyl-1,8-naphthyridines

AUTHOR(S): Rani, H. Shailaja; Mogilaiah, K.; Sreenivasulu, B.

CORPORATE SOURCE: Department Chemistry, Kakatiya University, Warangal, 506 009, India

SOURCE: Indian Journal of Heterocyclic Chemistry (1995), 5(1), 45-8

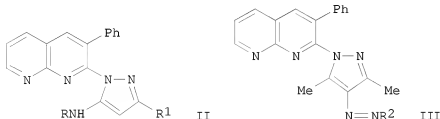
CODEN: IJCHEI; ISSN: 0971-1627

PUBLISHER: Lucknow University, Dep. of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB 2-Hydrazino-3-phenyl-1,8-naphthyridine (I) when heated with acetylacetone and Et acetoacetate gave 2-(3,5-dimethylpyrazol-1-yl)-3-phenyl-1,8-naphthyridine and 3-methyl-1-(3-phenyl-1,8-naphthyridin-2-yl)-5(4H)-pyrazolone. I was treated with acetoacetanilides/benzoylacetanilides and cyclized to give 2-(5-arylamino-3-methyl/phenylpyrazol-1-yl)-3-phenyl-1,8-naphthyridines II (R = Ph, substituted phenyl; R1 = Me, Ph). Cyclocondensation of I with arylazoacetylacetones gave the 2-(4-aryazo-3,5-dimethylpyrazol-1-yl)-3-phenyl-1,8-naphthyridines III (R2 = Ph, substituted phenyl). The compds. have been characterized on the basis of their elemental analyses and spectral data and tested for their antibacterial and antifungal activities.

IT 174137-80-5P

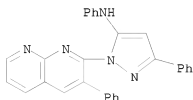
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and antimicrobial activity of some new 2-(pyrazol-1-yl)-1,8-naphthyridines)

RN 174137-80-5 HCAPLUS

CN 1H-Pyrazol-5-amine, N,3-diphenyl-1-(3-phenyl-1,8-naphthyridin-2-yl)- (CA INDEX NAME)



L4 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:217592 HCAPLUS

DOCUMENT NUMBER: 120:217592

ORIGINAL REFERENCE NO.: 120:38641a,38644a

TITLE: Synthesis and reactivity of 6H-1,3,4-selenadiazines

AUTHOR(S): Pfeiffer, W. D.; Rossberg, H.

CORPORATE SOURCE: Fachrichtung Chem., Ernst-Moritz-Arndt-Univ., Greifswald, Germany

SOURCE: Pharmazie (1993), 48(10), 732-5

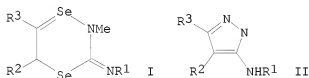
CODEN: PHARAT; ISSN: 0031-7144

Journal

DOCUMENT TYPE:

LANGUAGE: German

GI



AB The 6H-1,3,4-selenadiazines I [R1 = Pr, CHMe2, CMe3, Ph; R2 = H, Me, Ph; R3 = Me, Ph, 4-BrC6H4, 4-ClC6H4, 4-MeC6H4, 4-FC6H4] were prepared by condensation of α -halo ketones and H2NNMeCSeNHR1. I were converted to pyrazoles II by selenium elimination in boiling glacial acetic acid. Kinetic measurements show that I are much slower to undergo ring contraction than thiadiazines.

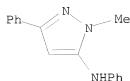
IT 153849-11-7P

RL: FORM (Formation, nonpreparative); PREP (Preparation)

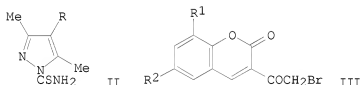
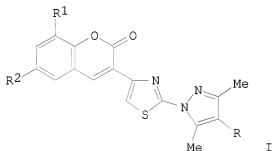
(formation of, by ring contraction of selenadiazine)

RN 153849-11-7 HCAPLUS

CN 1H-Pyrazol-5-amine, 1-methyl-N,3-diphenyl- (CA INDEX NAME)



L4 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1988:528892 HCAPLUS
 DOCUMENT NUMBER: 109:128892
 ORIGINAL REFERENCE NO.: 109:21473a,21476a
 TITLE: Studies on coumarin derivatives. Part V. Synthesis of a new type of pyrazolothiazole
 AUTHOR(S): Ravinder, P.; Rao, V. Rajeswar; Rao, T. V. Padmanabha
 CORPORATE SOURCE: Dep. Chem., Kakatiya Univ., Warangal, 506 009, India
 SOURCE: Collection of Czechoslovak Chemical Communications (1988), 53(2), 336-9
 CODEN: CCCCAK; ISSN: 0366-547X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 109:128892
 GI



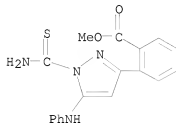
AB Eighteen of the title pyrazolothiazoles, e.g. I (R = H, PhN:N, 4-MeC6H4N:N, R1 = H, R2 = H, Br; same R, R1 = R2 = Br), were prepared in 70-80% yield by cyclocondensation of thiocarbamoylpyrazoles II with coumarins III.

IT 116317-18-1

RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclocondensation reaction of, with (bromoacetyl)coumarins, pyrazolothiazole derivs. from)

RN 116317-18-1 HCAPLUS

CN Benzoic acid, 2-[1-(aminothioxomethyl)-5-(phenylamino)-1H-pyrazol-3-yl]-, methyl ester (CA INDEX NAME)

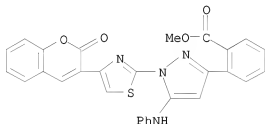


IT 116317-13-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and acetylation of)

RN 116317-13-6 HCAPLUS

CN Benzoic acid, 2-[1-[4-(2-oxo-2H-1-benzopyran-3-yl)-2-thiazolyl]-5-(phenylamino)-1H-pyrazol-3-yl]-, methyl ester (CA INDEX NAME)



L4 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1972:475162 HCAPLUS

DOCUMENT NUMBER: 77:75162

ORIGINAL REFERENCE NO.: 77:12419a,12422a

TITLE: Propiolamidines. I. Synthesis of N,N'-disubstituted phenylpropiolamidines and new routes to 5-N-substituted amino-3-phenylisoxazoles and 5-N-substituted amino-1,3-diphenylpyrazoles
Fujita, Hiroshi; Endo, Rokuro; Aoyama, Akira; Ichii, Takeshi

AUTHOR(S): Cent. Res. Lab., Sankyo Co., Ltd., Tokyo, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1972),

45(6), 1846-52
CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 77:75162

AB N, N'-Disubstituted phenylpropiolamidines were synthesized from phenylacetylene and carbodiimides. They were inert toward nucleophiles in a neutral or basic medium, but reactive in an acidic one. They reacted in

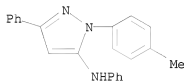
the presence of HCl with HONH₂, NH₂NH₂, and arylhydrazines to give 5-N-substituted amino-3-phenylisoxazoles, 5-N-substituted amino-3-phenylpyrazole and 5-N-substituted amino-1-aryl-3-phenylpyrazoles, resp., by nucleophilic addition followed by cyclization.

IT 36988-04-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 36988-04-2 HCAPLUS

CN 1H-Pyrazol-5-amine, 1-(4-methylphenyl)-N,3-diphenyl- (CA INDEX NAME)



L4 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1963:415565 HCAPLUS

DOCUMENT NUMBER: 59:15565

ORIGINAL REFERENCE NO.: 59:2795c-h,2796a-c

TITLE: Study of the β -oxo thioanilides. I. Reactions
with arylhydrazines

AUTHOR(S): Pocar, Donato; Bianchetti, Giuseppe; Maiorana, Stefano
UNIV. MILAN

CORPORATE SOURCE: Gazzetta Chimica Italiana (1963), 93, 100-13

SOURCE: CODEN: GCITA9; ISSN: 0016-5603

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB The reactions of PhNHNH₂ (I), p-O₂NC₆H₄NHNH₂ (II), oO₂NC₆H₄NHNH₂ (III), and 2,4-(O₂N)₂C₆H₄NHNH₂ (IV) with several β -oxo thioacid anilides yielded in all cases the corresponding arylhydrazones which frequently can be isolated in substance and then cyclized by various methods to pyrazoles. The tendency of the arylhydrazones to cyclize is correlated with the structural characteristics, such as steric hindrance and strain. It is demonstrated that the compound synthesized by Worrall (CA 14, 1832) and by Huenig, et al. (CA 57, 4653e), from I and BzSCH₂CO₂NHPh (V) is 1,3-diphenyl-5-phenylaminopyrazole (VI). V (2.55 g.) in 15 cc. 80% AcOH refluxed 4 hrs. with 1.08 g. I in 50% AcOH and evaporated gave VI, m. 153° (MeOH). 1,3-Diphenyl-2-methyl-5-chloropyrazole-HI (7.93 g.), 3.72 g. PhNH₂ heated 4 hrs. at 200° in a sealed tube also yielded VI. AcCH₂-CSNHPh (VII) (1.93 g.) in 20 cc. 70% AcOH treated with 1.08 g. PhNHNH₂, refluxed 2 hrs., cooled, and evaporated yielded the 3-Me analog of VI, m. 119-20°. 1-Cyclohexane-2-thiocarboxylic anilide (VIII) (2.33 g.) and 1.12 g. I mixed without solvent and diluted after a few min. with ligroine, and the oil layer washed with H₂O, dissolved with warming in EtOH, and cooled gave the phenylhydrazone (IX) of VIII, m. 138° (decomposition). IX refluxed 1 hr. in 90% AcOH (H₂S is evolved) yielded 2-phenyl-3-phenylamino-4,5,6,7-tetrahydroindazole (X), m. 158° (MeOH), also obtained by refluxing equimolar amts. of VIII and I during 2 hrs. in 60% AcOH. 1-Cyclopentanone-2-thiocarboxylic anilide (XI) (2.19 g.) in 10 cc. EtOH and 1.08 g. I kept at room temperature overnight yielded the phenylhydrazone (XII) of XI, m. 150-1° (decomposition) (EtOH). XII

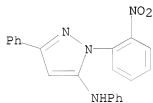
refluxed in AcOH gave 2-phenyl-3-phenylamino-4,5-dihydrocyclopenta[c]pyrazole (XIII), m. 148°, also obtained by heated equimolar amts. of I and XI in 60% AcOH during 3 hrs. V (5.1 g.) in 20 cc. EtOH treated with 3.06 g. II in 60 cc. hot 50% AcOH, refluxed 1 min., and filtered yielded the 1-(p-O2NC6H4) analog of VI, yellow crystals, m. 203°; the filtrate cooled yielded the red, crystalline 4-nitrophenylhydrazone of V, m. 200°, changing to yellow at 150-3°. VII (1.93 g.) in 10 cc. EtOH refluxed 0.5 hr. with 1.53 g. II in 50% AcOH and evaporated, the residue heated with 20% HCl, treated with C, and cooled, and the resulting 1-(p-nitrophenyl)-3-methyl-5-phenylaminopyrazole-HCl (XIV.HCl), pale yellow crystals, m. 188-93°, suspended in H2O, treated with aqueous K2CO3, and extracted with Et2O yielded XIV, light yellow, m. 111-12° (ligroine). VIII (2.33 g.) and 1.53 g. II in 50 cc. 50% AcOH heated 0.5 hr. yielded the 2-(p-O2NC6H4) analog of X, golden-yellow flakes, m. 135-6° (ligroine). XI (2.19 g.) and 1.53 g. II in 50 cc. 50% AcOH and 40 cc. EtOH refluxed 5 min. gave the p-nitrophenylhydrazone (XV) of XI, dark yellow needles, m. 160-1° (EtOH). XV and 1 equivalent Pb(OAc)2.3H2O in 50% AcOH refluxed 1 hr., filtered hot, and evaporated, and the residue washed with H2O, dissolved in Et2O, and evaporated gave the golden-yellow 1-(p-O2NC6H4) analog of XIII, m. 146-7° (ligroine). V (2.55 g.) in 10 cc. EtOH refluxed, treated with 1.53 g. III in 30 cc. 50% AcOH, refluxed 5 min., and worked up yielded the o-nitrophenylhydrazone (XVI) of V, m. 179° (decomposition) (EtOAc-petr. ether). XVI (3.90 g.) in 40 cc. AcOH treated with 3.80 g. Pb(OAc)2.3H2O in 15 cc. 50% AcOH, refluxed 0.5 hr., filtered, and diluted with an equal volume H2O yielded the yellow 1-(o-O2NC6H4) analog of VI, m. 164-5° (EtOH). VII (1.93 g.) in 10 cc. hot EtOH treated with 1.53 g. III in 25 cc. 50% AcOH and refluxed 5 min. yielded the orange o-nitrophenylhydrazone (XVII) of VII, m. 129-30° (EtOAc-petr. ether). XVII (3.28 g.) in 50 cc. AcOH refluxed 10 min. with 3.80 g. Pb(OAc)2.3H2O in 20 cc. 50% AcOH gave the yellow 1-(o-O2NC6H4) analog of VI, m. 130° (ligroine). VIII (2.33 g.) in 10 cc. EtOH refluxed 1 min. with 1.53 g. III in 30 cc. 50% AcOH yielded the yellow-orange o-nitrophenylhydrazone (XVIII) of VIII, m. 171-2° (EtOAc-petr. ether). XVIII (3.68 g.) in 100 cc. AcOH refluxed 20 min. with 3.80 g. Pb(OAc)2.3H2O in 20 cc. 50% AcOH gave the o-isomer of XIV, golden-yellow flakes, m. 165-6° (EtOH). XI (2.19 g.) in 20 cc. EtOH and 1.53 g. III in 40 cc. 50% AcOH refluxed 5 min. yielded the o-nitrophenylhydrazone of XI, red crystals, m. 118° (EtOH). V (2.55 g.) in 15 cc. EtOH and 1.98 g. IV in 50 cc. 70% AcOH refluxed 5 min. yielded the 2,4-dinitrophenylhydrazone (XIX) of V, m. 184° (decomposition) (EtOAc-petr. ether). XIX (2.17 g.) in 30 cc. AcOH refluxed 15 min. with 1.99 g. Pb(OAc)2.3H2O in 15 cc. 50% AcOH gave the 1-[2,4-(O2N)2C6H3] analog of VI, yellow-brown crystals, m. 216-17° (EtOH). VII (1.93 g.), 1.98 g. IV, and 30 cc. 60% AcOH, refluxed, diluted with EtOH to turbidity, refluxed 1 min., cooled, and filtered yielded the 2,4-dinitrophenylhydrazone (XX) of VII, golden-yellow flakes, m. 178-9° (EtOAc-Et2O). XX (3.73 g.) in 50 cc. refluxing AcOH treated with 3.80 g. Pb(OAc)2.3H2O in 15 cc. refluxing 50% AcOH, refluxed 15 min., filtered, and diluted with H2O, and the tacky precipitate dissolved in CHCl3

and

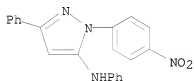
reptd. with petr. ether gave the 1-[2,4-(O2N)2C6H3] analog of XIV, dark orange needles, m. 156° (ligroine). VIII (2.33 g.) in 10 cc. EtOH refluxed with 1.89 g. IV in 40 cc. 70% AcOH, diluted with a few cc. EtOH to turbidity, and cooled after 20 min. yielded the golden-yellow 2,4-dinitrophenylhydrazone of VIII, m. 167° (EtOAc-petr. ether). XI

(2.19 g.) with 1.98 g. IV refluxed 10 min. in 15 cc. EtOH and 40 cc. 70% AcOH yielded the 2,4-dinitrophenylhydrazone of XI, yellow-orange crystals, m. 167° (EtOH).

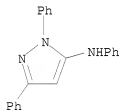
IT 88844-15-9P, Pyrazole, 5-anilino-1-(o-nitrophenyl)-3-phenyl-
 88844-16-0P, Pyrazole, 5-anilino-1-(p-nitrophenyl)-3-phenyl-
 94863-16-8P, Pyrazole, 5-anilino-1,3-diphenyl- 94878-85-0P
 , Pyrazole, 5-anilino-1-(2,4-dinitrophenyl)-3-phenyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 88844-15-9 HCAPLUS
 CN 1H-Pyrazol-5-amine, 1-(2-nitrophenyl)-N,3-diphenyl- (CA INDEX NAME)



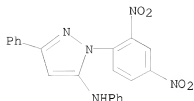
RN 88844-16-0 HCAPLUS
 CN 1H-Pyrazol-5-amine, 1-(4-nitrophenyl)-N,3-diphenyl- (CA INDEX NAME)



RN 94863-16-8 HCAPLUS
 CN 1H-Pyrazol-5-amine, N,1,3-triphenyl- (CA INDEX NAME)



RN 94878-85-0 HCAPLUS
 CN 1H-Pyrazol-5-amine, 1-(2,4-dinitrophenyl)-N,3-diphenyl- (CA INDEX NAME)



L4 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1963:33419 HCAPLUS

DOCUMENT NUMBER: 58:33419

ORIGINAL REFERENCE NO.: 58:5692b-g

TITLE: Ketene derivatives. V. Oxalylketene mercaptals and related compounds

AUTHOR(S): Stachel, Hans Dietrich

CORPORATE SOURCE: Univ. Marburg, Germany

SOURCE: Chemische Berichte (1962), 95, 2166-71

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 58:33419

GI For diagram(s), see printed CA Issue.

AB cf. CA 58, 4540b. [(EtO)2C:CHCO]2 (I) was converted with suitable mercaptans to oxalylketene O,S-acetals or oxalylketene mercaptals which were also prepared from CH2:C(OEt)SEt (II) or CH2:C(SET). (III), resp., with (COCl)2 (IV). I (1.4 g.) and 3 cc. PhCH2SH heated slowly to about 170°, kept several min. at 175°, cooled, diluted with 4 vols. EtOH, and filtered after 0.5 hr. gave 1.1 g. yellow [OCCH:C(OEt)SCH2Ph]2 (V), decomposed about 190°. V and piperidine refluxed 2 min. gave yellow oxalylketene tetrapiperidinoaminal. II (3.1 g.) in 15 cc. dry Et2O treated at 0° with 0.5 cc. IV, kept 15 min. at room temperature, and filtered gave 0.9 g. yellow [OCCH:C(OEt)SEt]2 (VI), m. 154-5°. VI (0.2 g.) shaken with EtOH and kept 5 days at room temperature with an equal weight

PhNH2 gave yellow oxalylketene dianilino-O,N-acetal (VII), m. 160-2° (Ac2O). VI (0.5 g.) in EtOH and 5 drops concentrated HCl kept 3 days and evaporated at room temperature gave (COCH2CO2Et)2, m. 78-80°. I (1.4 g.) and 2 cc. (CH2SH)2 warmed to beginning reaction, diluted after 2-3 min. with 2 vols. EtOH, and filtered after 0.5 hr. yielded 0.3 g. yellow oxalylketene bis(ethylene)mercaptopal, m. 260° (decomposition) (2:1 AcOH-HCONMe2). (EtS)2C:CHCOCOCl (VIII) (2.4 g.) in 120 cc. dry Et2O treated with 3.7 g. III and kept 24 hrs. at room temperature yielded 0.9-1.0 g. [OCCH:C(SET)2]2 (IX), m. 160-1° (Ac2O). VIII (2.4 g.) in about 10 cc. dry Et2O and 3.0 g. III kept overnight and filtered gave 75 mg. IX; the filtrate cooled gave 1.3 g. EtSCOCOCH:C(SET)2 (X). VIII (2.4 g.) added to 3.7 g. III and 1.27 g. iodine in 20 cc. dry Et2O, kept 24 hrs. at room temperature, filtered, and the residue treated dropwise with piperidine left 0.65 g. IX undissolved; the mother liquor cooled gave 1.1 g. mixture of VIII and X. II (1.5 g.) in 5 cc. dry Et2O treated at -50° with 0.5 cc. IV and filtered, the residue added to excess CH2N2-Et2O, the mixture evaporated, and the crude product dissolved in a few cc. Et2O, filtered from the insol. polymethylene, and cooled to -50° gave 150 mg. yellow EtS(EtO)C:CHCOCOCHN2, m. 100-1°. VIII (0.5 g.) warmed briefly in H2O-containing dioxane and evaporated yielded 0.35 g. yellow (EtS)2C:CHCOCO2H,

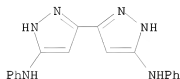
m.

about 125° (decomposition) (iso-Pr₂O), which with CH₂N₂ gave the Me ester. IX (0.5 g.) in about 10 cc. boiling PrOH treated dropwise with 0.5 g. N₂H₄.H₂O, refluxed about 15 min., and evaporated gave 250 mg. brownish yellow XI, m. 155-6° (MeOH). VII (0.5 g.) in PrOH treated dropwise with 10 drops N₂H₄.H₂O, heated about 3 min., filtered, and cooled gave 200 mg. red 3,3'-bis(5-anilinopyrazole), m. 265-8° (1:1 HCONMe₂-H₂O). III in EtOH with ale. iodine yielded black, powdery III.I₂, decomposed 85-90°.

IT 98494-86-1P, 3,3'(or 5,5')-Bipyrazole, 5,5'(or 3,3')-dianilino-
 RL: PREP (Preparation)
 (preparation of)

RN 98494-86-1 HCAPLUS

CN [3,3'-Bi-1H-pyrazole]-5,5'-diamine, N5,N5'-diphenyl- (CA INDEX NAME)



=> log y

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

93.21	279.31
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-11.48	-11.48

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